

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

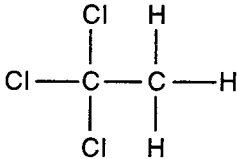
Information regarding the chemical identity of 1,1,1-trichloroethane is located in Table 3- 1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1 ,1 ,1 -trichloroethane is located in Table 3-2.

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TABLE 3-1. Chemical Identity of 1,1,1-Trichloroethane

Characteristic	Information	Reference
Chemical name	1,1,1-Trichloroethane	CAS 1994
Synonym(s)	Methylchloroform	CAS 1994
	Methyltrichloromethane	SANSS 1994
	Trichloromethylmethane	
	α-Trichloromethane	
Registered trade name(s)	Chlorothene NU	OHM-TADS 1994
	Aerothene TT	
Chemical formula	CCl ₃ CH ₃	CAS 1994
Chemical structure		
Identification numbers:		
CAS registry	71-55-6	CAS 1994
NIOSH RTECS	KJ2975000	RTECS 1994
EPA hazardous waste	U226	HSDB 1994
OHM/TADS	8100101	OHM/TADS 1994
DOT/UN/NA/IMCO shipping	UN 2831	HSDB 1994
HSDB	157	HSDB 1994
NCI	C04626	HSDB 1994

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/ North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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TABLE 3-2. Physical and Chemical Properties of 1,1,1-Trichloroethane

Property	Information	Reference
Molecular weight	133.4	CAS 1993
Color	Colorless	Archer 1979; Sax and Lewis 1987
Physical state	Liquid	Merck 1989
Melting point	-30.4 °C -33.0 °C	Weast 1988 Archer 1979
Boiling point	74.1 °C	Merck 1989
Density:		
at 20 °C	1.3390 g/mL	Weast 1988
at 25 °C	1.3299 g/mL	Riddick et al. 1986
at 30 °C	1.32096 g/mL	Riddick et al. 1986
Odor	Ethereal, chloroform-like	Archer 1979; Aviado et al. 1976
Odor threshold:		
Water	No data	
Air	120 ppm 500 ppm	Amoore and Hautala 1983; Reist and Rex 1977
Solubility:		
Water at 20 °C	0.1495% (wt/wt)	Horvath 1982
Organic solvent(s)	Soluble in alcohol, ether, chloroform; miscible with other chlorinated solvents; soluble in common organic solvents	Weast 1988; Archer 1979
Partition coefficients:		
Log K _{ow}	2.49	Hansch and Leo 1985
Log K _{oc}	2.03 2.02	Friesel et al. 1984 Chiou et al. 1979
Vapor pressure at 20 °C	124 mm Hg 16.4 kPa	Boublik et al. 1984 Riddick et al. 1986
Henry's law constant:		
at 20 °C	6.3x10 ⁻³ atm-m ³ /mol	Chiou et al. 1980
at 30 °C	17.2x10 ⁻³ atm-m ³ /mol	Gossett 1987
Autoignition temperature	537 °C	HSDB 1992
Flashpoint	None	Archer 1979
Flammability limits	8–10.5%	Archer 1979
Conversion factors		
ppm (v/v) to mg/m ³ in air (20 °C)	1 ppm = 5.4 mg/m ³	Chiou et al. 1980
mg/m ³ to ppm (v/v) in air (20 °C)	1 mg/m ³ = 0.185 ppm	
Explosive limits	7.5–12.5% in air	NIOSH 1990

CAS = Chemical Abstracts Services; HSDB = Hazardous Substances Data Bank; NIOSH = National Institute for Occupational Safety and Health; v/v = volume by volume; wt/wt = weight by weight